CONF-860132--2

FLUID FLOW AND HEAT TRANSFER MODELING FOR CASTINGS

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CONF-860132--2

DE85 007999

Abstract

Casting is fundamental to manufacturing of many types of equipment and products. Although casting is a very old technology that has been in existence for hundreds of years, it remains a highly empirical technology, and production of new castings requires an expensive and time-consuming trial-and-error approach.

In recent years, mathematical modeling of casting has received increasing attention; however, a majority of the modeling work has been in the area of heat transfer and solidification. Very little work has been done in modeling fluid flow of the liquid melt. This paper presents a model of fluid flow coupled with heat transfer of a liquid melt for casting processes. The model to be described in this paper is an extension of the COMMIX code and is capable of handling castings with any shape, size, and material. A feature of this model is the ability to track the liquid/gas interface and liquid/solid interface. The flow of liquid melt through the sprue and runners and into the mold cavity is calculated as well as three-dimensional temperature and velocity distributions of the liquid melt throughout the casting process.

MASTER

Presented at

Modeling and Control of Casting and Welding Processes

Santa Barbara, California

January 12-17, 1986

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Introduction

Bower et al. (1), in their 1969 review of the evolution of some of the casting techniques, stated that:

> "The evolution of technology requires alternatives to be available so that choices can be made that lead to changes. The role of solidification science and other disciplines related to casting technology is to develop a better understanding of process and product, so that a wider range of alternatives is possible.
>
> Alternatives, whether from science or from invention, must lead to improvements in casting "utility." Utility, or economic advantage, must include consideration of total system costs, and final product value. The cost of materials, melt processing and finishing should be optimized with casting costs, since all are part of the production system. It is the favorable relationship between total processing costs and product value that makes a change in casting technology viable, but the best change is not possible unless technology has provided an understanding."

In the above paragraphs, twice did Bower et al. mention the word understanding as a basis for technology evolution. Technological understanding in general (and for casting in particular) may be gained through empirical means, i.e., trial and error, which is often costly and time consuming. An effective means for gaining scientific understanding is to utilize first-principle, physics based mathematical modeling techniques, coupled with experimental modeling (2) and verification. The utility and advantage of this latter approach need not be advocated at this symposium since most participants are already experienced practitioners of modeling principles. The multitude of the symposium session topics also attests to the fact that both casting and welding involve several major disciplinary sciences/engineerings (e.g., fluid mechanics, heat transfer, solidification, metallurgy and microstructure, continuum mechanics, deformation processing, etc.), and that Flemings' suggestion of component modeling and final synthesis (2) may indeed by necessary due to the complexity of the problem.

While much work has been done in the past on heat transfer and solidification modelings, advanced fluid-flow modeling of casting has received attention only in recent years (2-4). The benefits resulting from the study of fluid flow in the casting process are: (a) to control and possibly eliminate cold shot, erosion of mold, and porosity problem associated with entrainment of air or other types of gases in the mold and surface, (b) to provide a better understanding of microstructure of a casting as a result of the fluid flow pattern and heat transfer during solidification. Among the casting areas where fluid flow coupled with heat transfer modeling plays an important role may include (a) free surface, liquid-melt filling of cavity molds of complex shapes, (b) free convective flow in liquid melt, (c) convective flow in liquid melt induced by external forces (e.g., electromagnetic stirring), and (d) eddy currents/magnetic pressure encountered in electromagnetic (EM) levitation casting. The last area of EM casting is currently being pursued at Argonne National Laboratory in an effort to develop a continuous casting process for near net shape forming of sheet steels. This work is part of the U.S. Steel Initiative with industry/national-laboratory collaboration. The work at Argonne involves design/construction of an EM continuous casting facility which also embodies a modeling task to provide the needed analytical

This paper is primarily concerned with the fluid flow and heat transfer modeling for castings. A computer program, COMMIX (COMponent MIXing) (5-7), is the basic tool used for generating the results in this paper. COMMIX is a fully three-dimensional, steady-state/transient, single-/multi-species, and single-/multiphase code for thermal hydraulic analysis of single- and multi-component systems. Approximately 10 million U.S. dollars have been spent in its development and the code is currently being used worldwide at over 50 installations, mostly by nuclear-reactor related establishments. Among the unique features of COMMIX, the new porous-medium formulation (8-10) is perhaps the most significant. With this formulation and its associated parameters of volume porosity, directional surface porosity, distributed resistance and distributed heat source or sink, COMMIX can, for the first time and in a unified and consistent manner, model anisotropic flow and temperature fields with stationary structures, as well as simulate multidimensional thermal hydraulic environment of either a single component (e.g., fuel rod bundle, heat exchanger, etc.), or a multicomponent system that is a combination of these components.

The COMMIX code is being developed primarily for liquid sodium and water which are coolants for liquid metal fast breeder reactors and light water reactors respectively. Governing equations, solution techniques, and unique features of COMMIX will be described to acquaint readers with the code. Preliminary modification of COMMIX has been completed so that the code can now handle fluid flow and heat transfer aspects of casting and solidification. Initial case studies to be presented in this paper made use of a model system (water/ice) to demonstrate the COMMIX capabilities. A brief synopsis is given at the end that also covers our planned future activities.

Mathematical Model

A system of conservation equations of mass, momentum, and energy is derived via local volume averaging, and solved numerically by the COMMIX code as a boundary value problem in space and an initial value problem in time. A two-equation k-ε turbulent model is provided as user's option where k is a turbulence kinetic energy and ε is the dissipation rate of k. All these equations are described separately as follows:

Conservation of Mass

$$\gamma_V \frac{\partial \rho}{\partial t} + \nabla \cdot \gamma_A \rho \underline{u} = 0 \tag{1}$$

where ρ = density,

$\underline{u}$ = velocity vector,

t = time,

γ_V = volume porosity which is the ratio of the volume occupied by fluid in a control volume to the total control volume,

γ_A = directional surface porosity is the ratio of the flow area in a control surface at a given direction to the total control surface in that direction,

$$\nabla = \frac{\partial}{\partial x}\underline{i} + \frac{\partial}{\partial y}\underline{j} + \frac{\partial}{\partial z}\underline{k}$$

x, y, z = principal directions in Cartesian coordinates, and

$\underline{i}, \underline{j}, \underline{k}$ = unit vector in the x, y, and z direction, respectively.

Conservation of Momentum

$$\gamma_v \frac{\partial \rho \underline{u}}{\partial t} + \nabla \cdot \gamma_A \rho \underline{u}\underline{u} = -\gamma_v \nabla P + \nabla \cdot \gamma_A \underline{\underline{\tau}} + \gamma_v \left(\rho \underline{g} - \underline{R}\right) \tag{2}$$

where P = pressure,

$\underline{\underline{\tau}}$ = viscous stress tensor,

$\underline{g}$ = gravitational acceleration, and

$\underline{R}$ = distributed flow resistance.

Conservation of Energy in Terms of Enthalpy

$$\gamma_v \frac{\partial \rho h}{\partial t} + \nabla \cdot \gamma_A \rho h \underline{u} = \gamma_v \frac{dP}{dt} - \nabla \cdot \gamma_A \kappa \nabla T + \gamma_v \left(J_E + \phi + \dot{Q}_w\right) \tag{3}$$

where κ = conductivity

T = temperature

J_E = heat source

ϕ = dissipation rate per unit volume, and

$\dot{Q}_w$ = heat transfer rate at wall.

Turbulent Transport Equations

Transport Equation for k (Turbulent Kinetic Energy)

$$\frac{\partial \rho k}{\partial t} + \nabla \cdot \rho \underline{u} k = P_k + G_k - \rho \varepsilon + \nabla \cdot \left(\frac{\mu_{tur} + \mu_{lam}}{\sigma_k}\right) \nabla k \tag{4}$$

where $P_k = \mu_{tur} \left[\frac{\partial u_i}{\partial x_j} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right]$

$G_k = -\frac{\mu_{tur}}{\rho \sigma_k} \frac{\partial f}{\partial T} \left(\frac{\partial T}{\partial x_j} g_j\right)$

μ_{tur} = turbulent viscosity = $\frac{C_D \rho k^2}{\varepsilon}$

μ_{lam} = molecular or laminar viscosity,

σ_k = turbulent Prandtl number for k

C_D = empirical coefficient (recommended value is 0.09).

Transport Equation for ε (Dissipation rate of k)

$$\frac{\partial \rho \varepsilon}{\partial t} + \nabla \cdot \rho \underline{u}t = C_1 \frac{\varepsilon}{k}\left(P_k + G_k\right) - C_2 \frac{\rho \varepsilon^2}{k} + \nabla \cdot \left(\frac{\mu_{tur} + \mu_{lam}}{\sigma_\varepsilon}\right)\nabla \varepsilon \qquad (5)$$

where σ_ε = turbulent Prandtl number for ε

C_1, C_2 = empirical coefficients (recommended values are 1.44 and 1.92 respectively)

Equations 1 through 5 are solved with a set of appropriate initial and boundary conditions which are detailed in Ref. 6. Two solution procedures, modified ICE (11) and modified SIMPLER (12), are provided as user's options.

Unique Features of the COMMIX Code

The following are unique features of the COMMIX code (7).

- **New Porous-Medium Formulation:** COMMIX uses a new porous-medium formulation with the parameters volume porosity, directional surface porosity, distributed resistance, and distributed heat source or sink. With this formulation, the COMMIX code has the capability to model anisotropic flow and temperature fields with stationary structures. The porous-medium formulation with the additional parameter of directional surface porosity represents a unified approach to thermal-hydraulic analysis. Because of this feature, it is now possible to perform a multidimensional thermal-hydraulic simulation of either a single component, such as a rod bundle, reactor plenum, piping system, heat exchanger, etc., or a multicomponent system that is a combination of these components. This new porous medium formulation is particularly useful in simulating irregular geometries.

- **Two Solution Procedures:** In COMMIX, two solution procedures, semi-implicit and fully implicit, are available as a user's option. The semi-implicit procedure, a modification of the ICE technique, is designed for fast transient analysis, where the interest is to examine flow phenomenon in the time period of the order of Courant time step size. The fully implicit procedure, named SIMPLEST-ANL and similar to the SIMPLE/SIMPLER algorithms, is designed for normal and slow transients, where the interest is to examine phenomena at times that are larger than Courant time step size.

- **Geometrical Package:** A special geometrical package has been developed and implemented that permits modeling of any complex geometry in the most storage-efficient way.

- **Skew-Upwind Difference Scheme:** A new volume-weighted skew-upwind difference scheme has been developed and implemented that reduces numerical diffusion observed in simulations of flow inclined to grid lines. The scheme also eliminates temperature over/undershoots that are found to occur when simulations are performed with normal skew-upwind differencing schemes.

- **Turbulence Modeling:** The following four turbulence model options are provided to give COMMIX-1B (a derivative of COMMIX) a wide range of applications:

  - Constant turbulent diffusivity model

  - Zero-equation mixing length model

  - One-equation (k) model

  - Two-equation ($k-\varepsilon$) model

- **Generalized Resistance and Thermal Structure Model:** The COMMIX code also contains: (a) a generalized resistance model to permit specification of resistance due to internal structures, and (b) a generalized thermal structure formulation to model thermal interaction between structures (casting mold wall) and surrounding fluid.

- **Modular Structure:** The code is modular in structure, which expedites rapid implementation of the latest available drag models, heat-transfer models, etc. It also permits solution of 1D, 2D, or 3D calculations.

Free Surface Flow

To use the COMMIX code to model the filling of a mold, an additional capability for free surface flow must be added for a given mold configuration which is subdivided into a number of computational cells. These Eulerian cells remain fixed in space and have a temperature, pressure, velocity, etc. associated with each of them. In addition to the standard variables, a variable F (fractional volume of fluid) (13) is introduced for each cell to keep track of fluid, interface, and empty regions within the configurations, where $F = 1$ indicates a cell full of fluid, $F = 0$ indicates an empty cell. At any given time, the variable F can be scanned over the configuration and each cell classified as being

1. Full - cells containing fluid and bounded only by other full and surface cells.

2. Empty - cells with no fluid and bounded only by other empty and surface cells.

3. Surface - interface cell, bounded by other surface, full, and at least one empty cell.

The governing equation for F (fractional volume of fluid) (13) is

$$\frac{\partial F}{\partial t} + \bar{v} \cdot \bar{\nabla} F = 0 , \qquad (6)$$

which implies that F is a quantity that moves with the fluid. In discretizing the above equation, several physical and numerical constraints must be observed:

1. The value of F must be between 0 and 1 inclusive. A cell cannot be less than empty or more than full.

2. Fluid cannot be transported through more than one cell during a time step. This gives rise to the Courant time step limitation that

$$\Delta t \sim < \left|\frac{\Delta x}{U}\right|_{\min} \qquad (7)$$

3. A full cell stays full if only surrounded by other full cells. Since a full cell is next to only other full cells and surface cells, the only way F can change is if a void is convected in from an adjacent surface cell which has just emptied.

4. An empty cell remains empty if surrounded only by other empty cells. Since an empty cell is adjacent to only other empty and surface cells, the only way F can change is if fluid is convected in from an adjacent surface cell which has just filled.

5. A cell containing an interface can be either filling or emptying. However, if a surface cell becomes full during a time step, any fluid excess will convect to adjacent empty cells. Conversely, if a surface cell empties, any additional void will convect into adjacent full cells.

The velocity field is determined in the standard way between cells containing some fluid (surface and full cells). Interface boundary conditions are used to set the velocity between surface and empty cells. No velocity calculation is needed between empty cells. In consideration of rules 1 through 5 above, it is seen that no calculation of F is needed in empty cells surrounded by other empties or fulls surrounded by other fulls. Indeed, no fractional volume of fluid calculation need be done except in cells containing an interface. Adjustments to adjacent full or empty cells are made only when considering surface cells which have either been filled or emptied respectively.

Isolating the F calculation to cells containing an interface and bypassing the calculation for full and empty cells substantially reduces the number of calculations required for tracking the interface and represents a departure from the standard VOF method (14). This reduction is particularly important in 3-D analyses for which the vast majority of cells are away from the interface.

The above method provides a very effective and economical technique for tracking the fluid interface. Work is continuing to couple all the features of the COMMIX code to the interface tracking technique. When completed, a code with synergistic features is expected which can give new insights into the casting process.

Results

Typical results obtained from the COMMIX code for mold filling are shown in Figs. 1 through 9. Figure 1 presents the dimensions of the mold and the COMMIX computational mesh set-up. Figures 2 through 9 show the time sequence of liquid melt filling the mold cavity. In this particular numerical simulation, the liquid melt was assumed isothermal with self-replenishment to maintain constant elevation at A-A as shown in Fig. 1. A diaphragm is located at elevation B-B which was breached at $t = 0$ and the liquid melt rushes into the cavity where t stands for time. Figures 10 through 13 present the sequence of solidification configurations of the liquid melt as a function of time. In this calculation, it was assumed that (a) the fluid is water/ice, (b) a single value enthalpy determines state, (c) the initial water temperature is 10°C, and (d) at time = 0, all walls drop to -40°C. Similar work (4) on mold filling was presented in this meeting; however, it was limited to two-dimensional analyses.

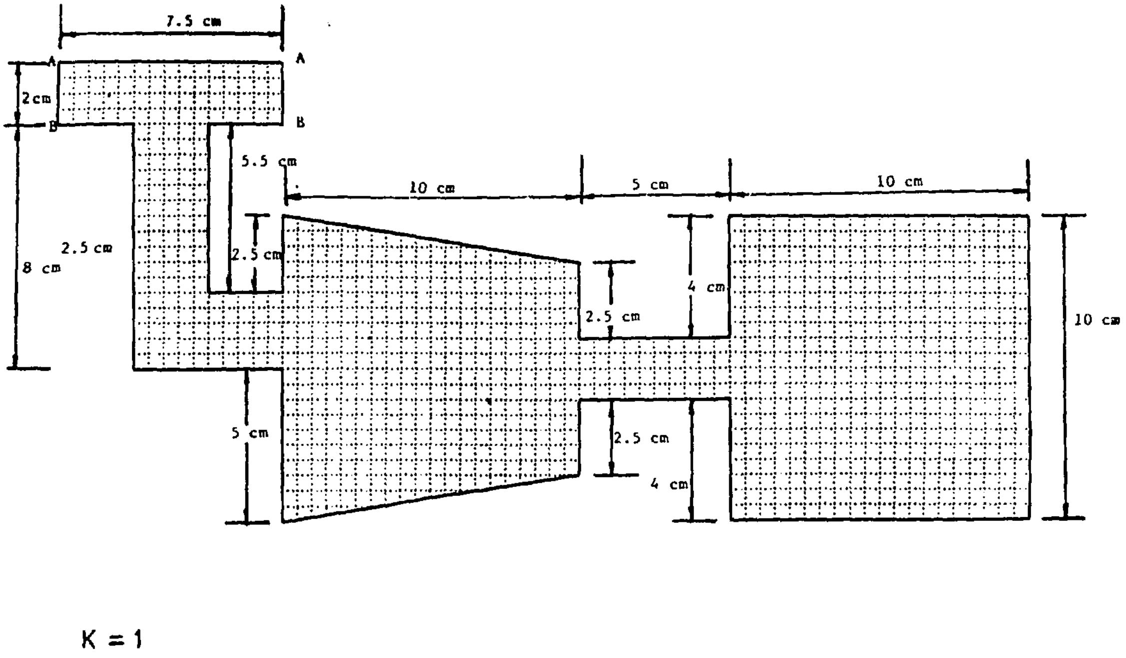

Figure 1 - Computational Mesh Set-up and Dimensions

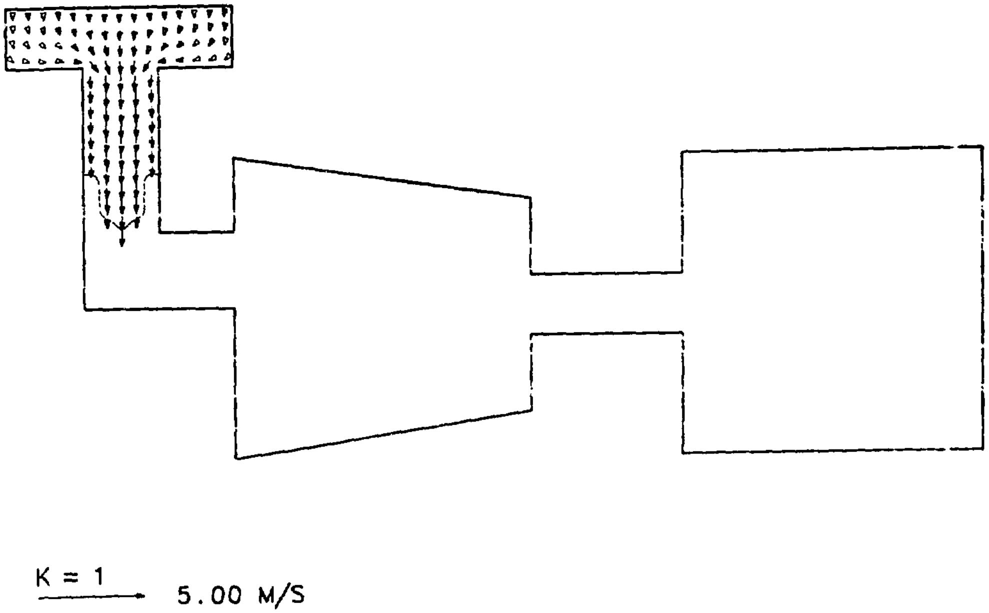

Figure 2 - Mold Filling at time = 0.10 s

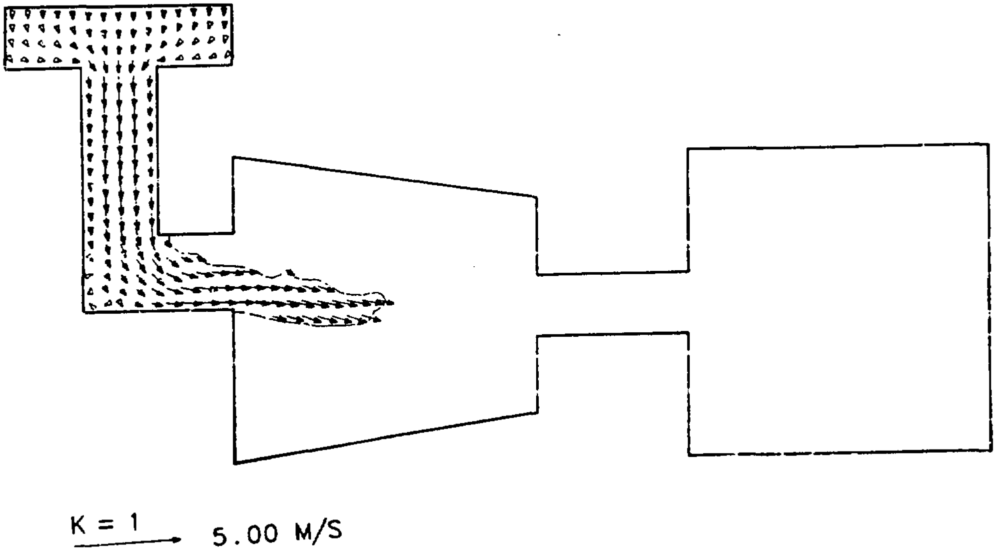

Figure 3 - Mold Filling at time = 0.20 s

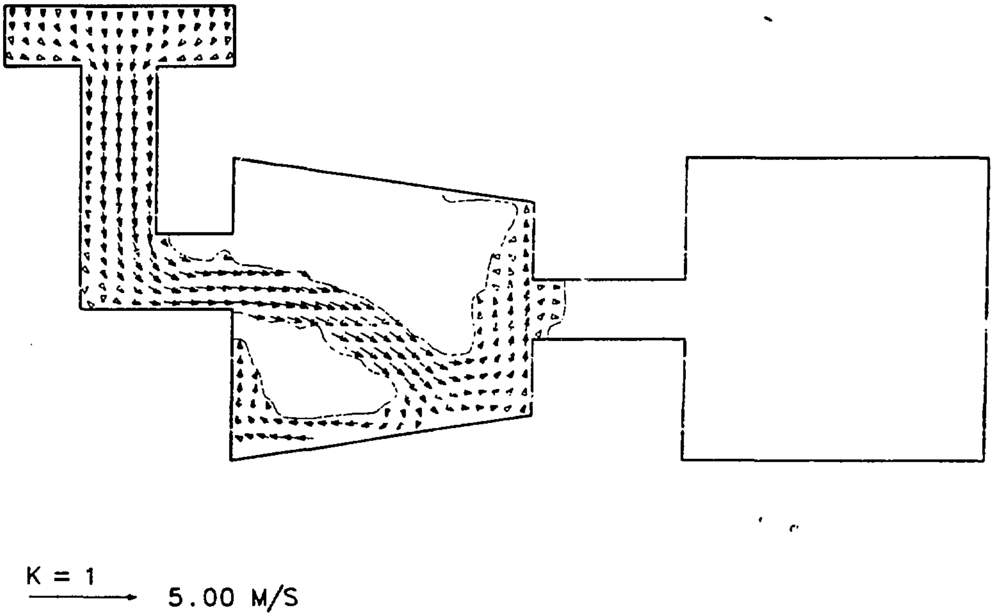

Figure 4 - Mold Filling at time = 0.40 s

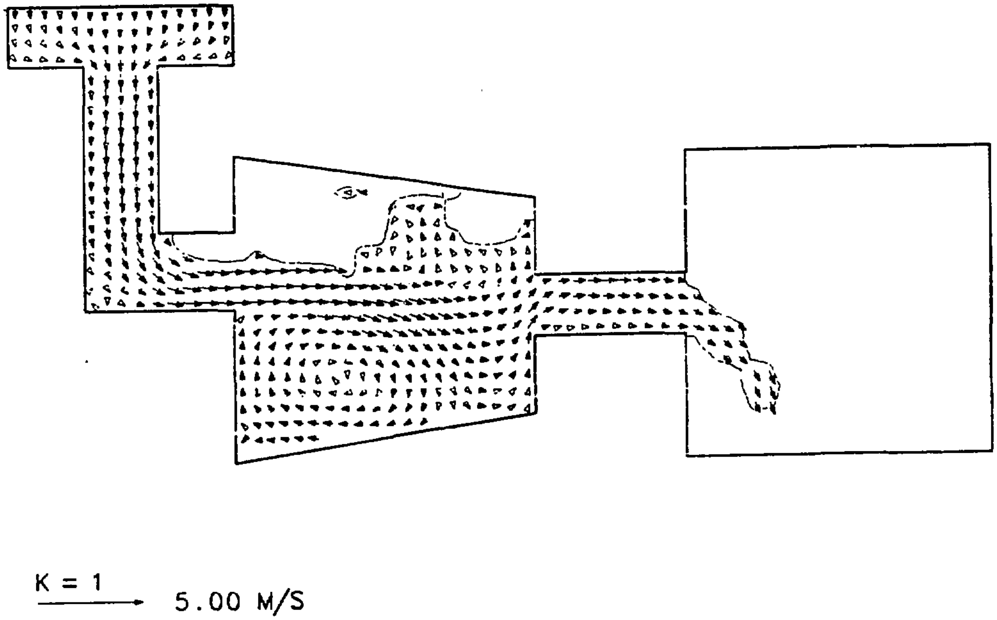

Figure 5 - Mold Filling at time = 0.60 s

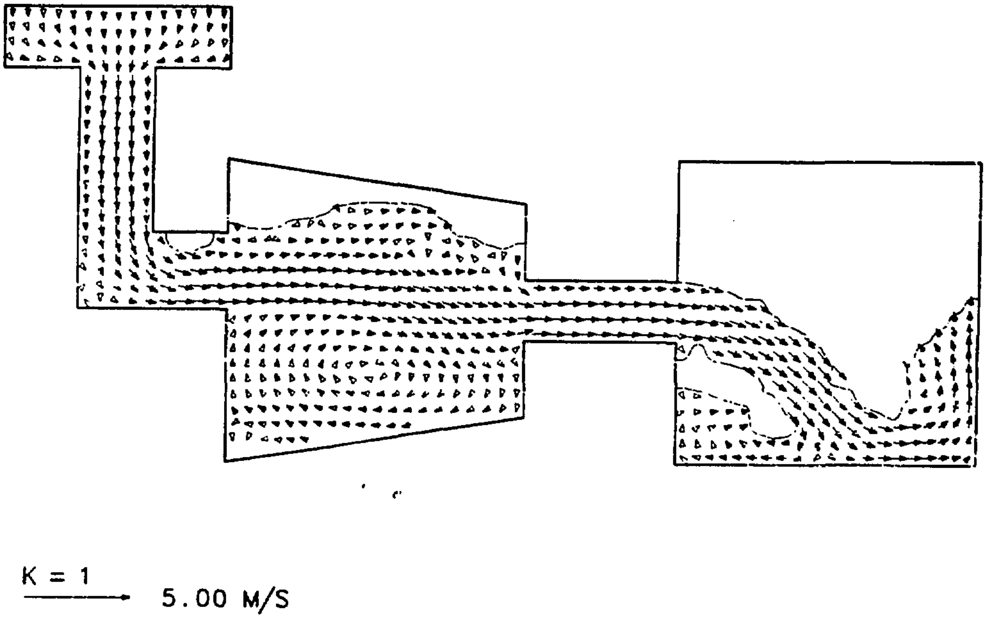

Figure 6 - Mold Filling at time = 0.80 s

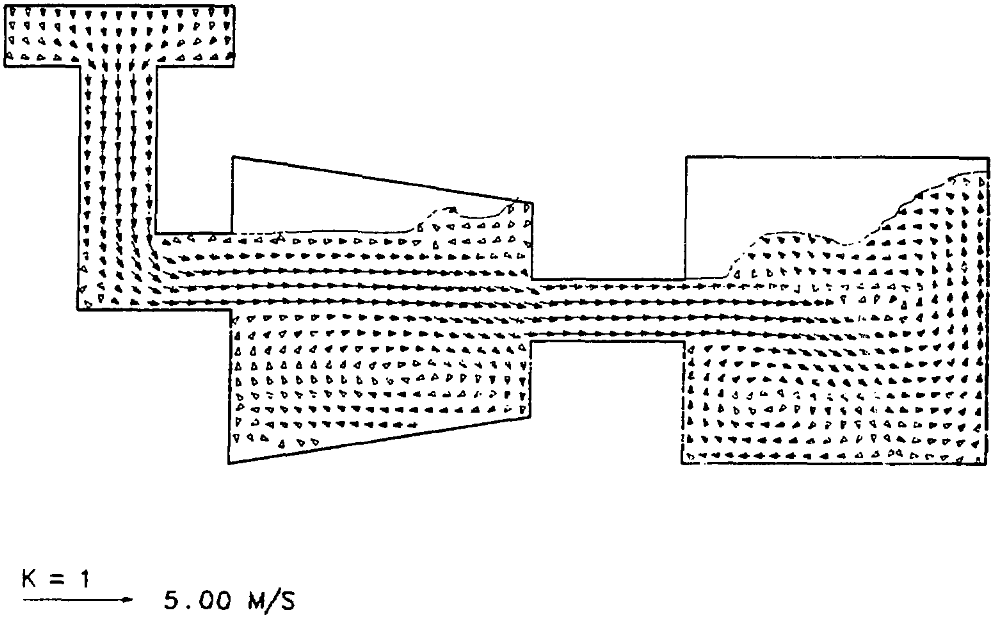

Figure 7 - Mold Filling at time = 1.00 s

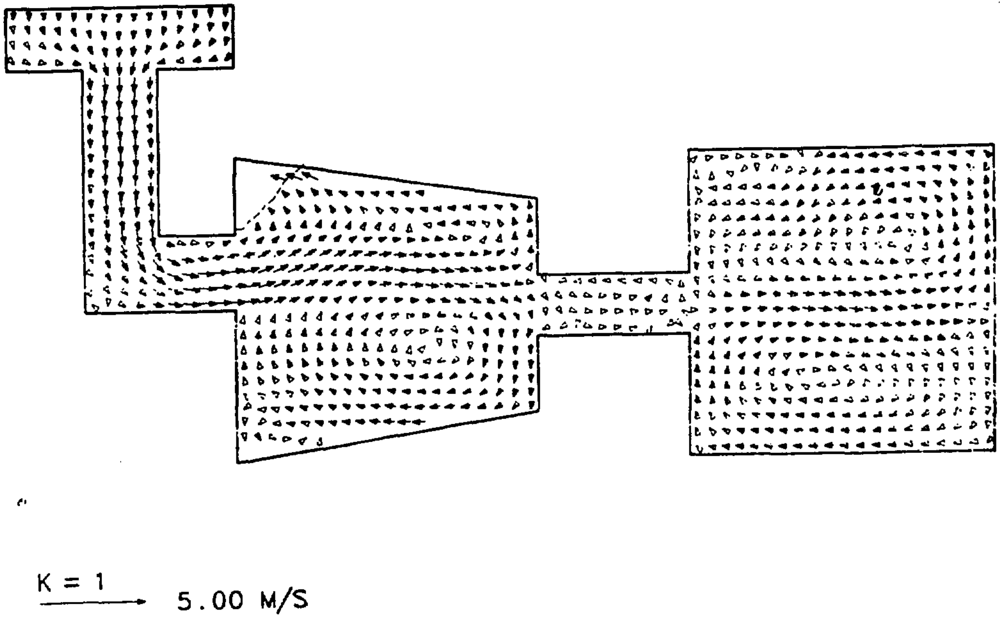

Figure 8 - Mold Filling at time = 1.20 s

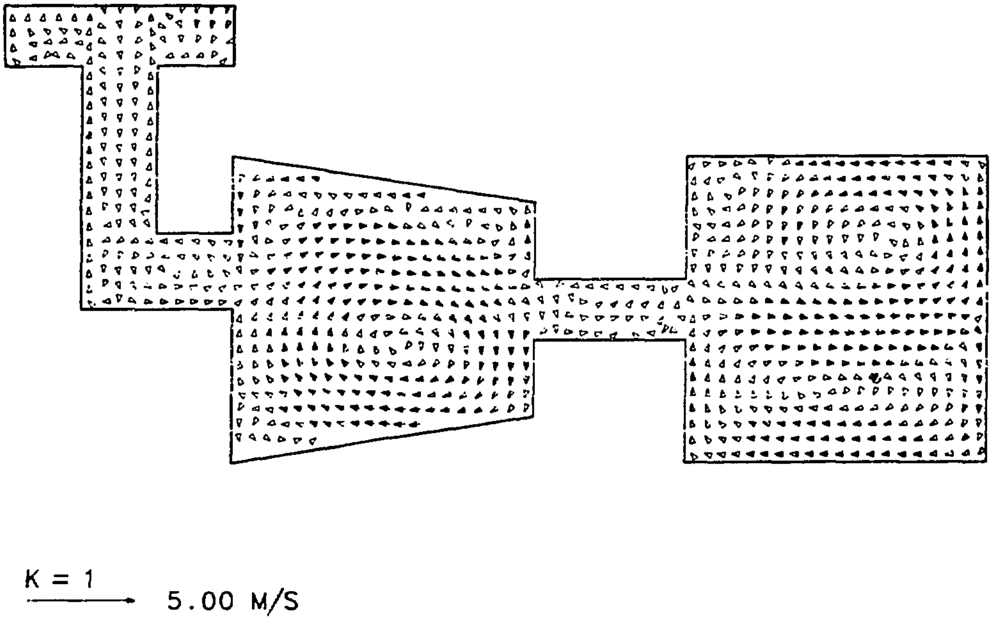

Figure 9 - Mold Filling at time = 1.30 s

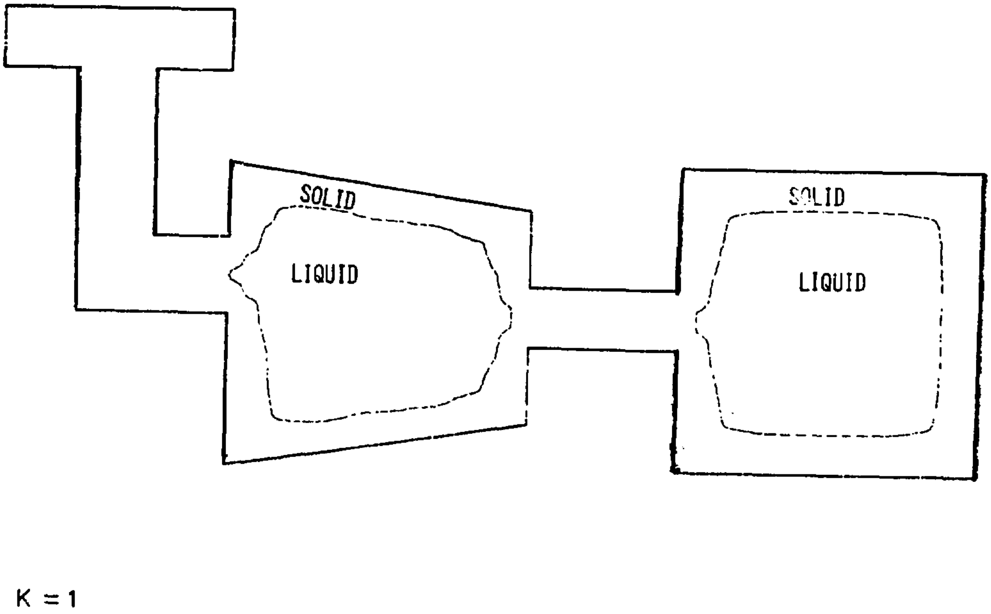

Figure 10 - Solidification at time = 1660.0 s

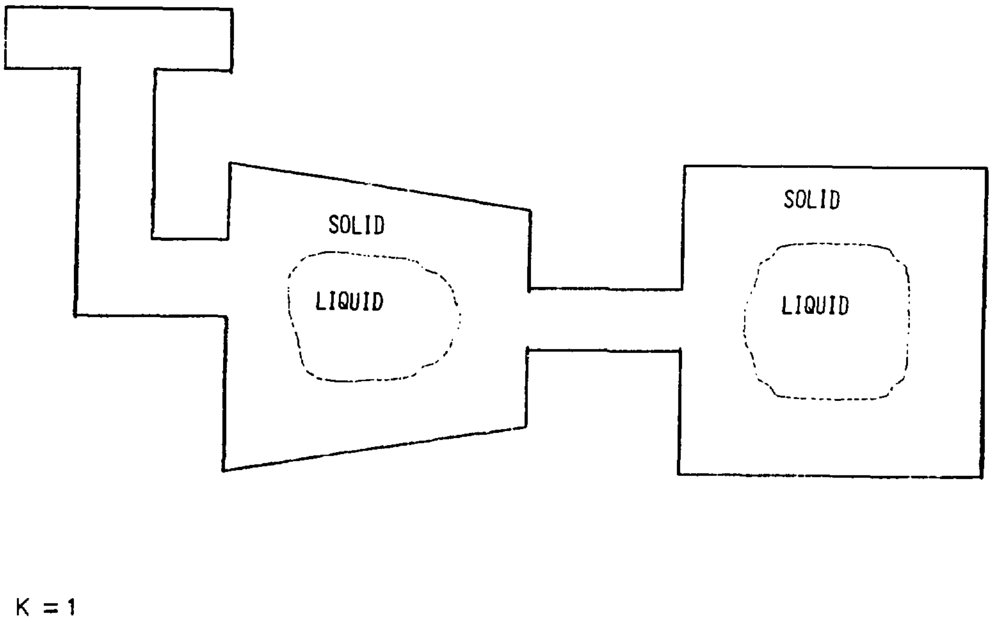

Figure 11 - Solidification at time = 5040.0 s

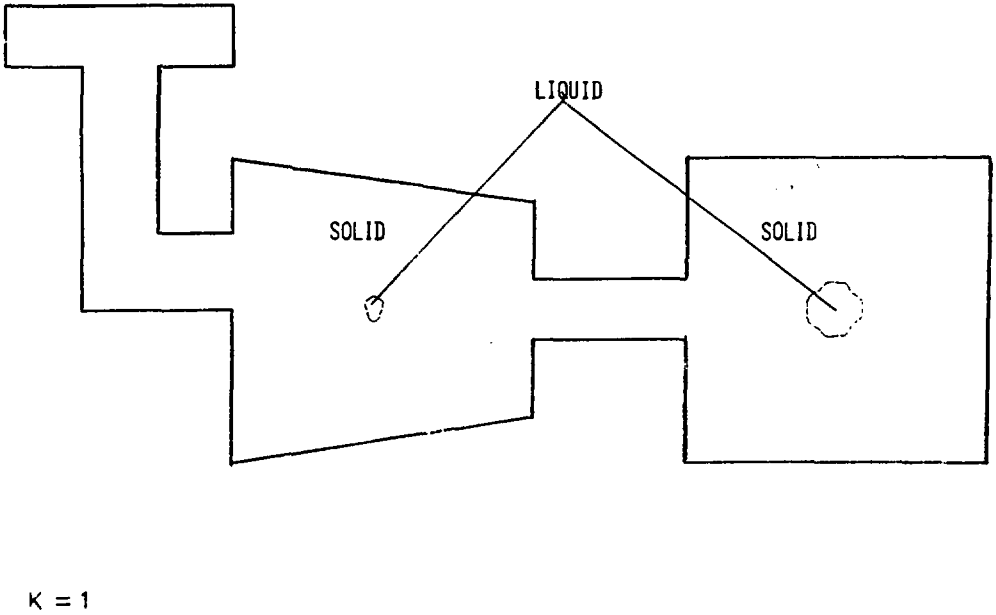

Figure 12 - Solidification at 10580.0 s

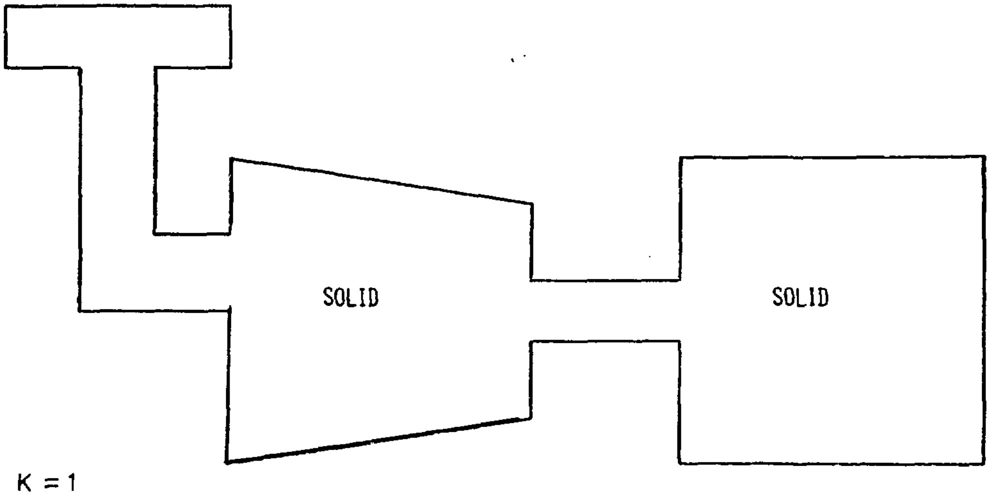

Figure 13 - Solidification at 12300.0 s

Discussions and Conclusions

Although water/ice has been used to demonstrate COMMIX capabilities, it should be noted that the governing equations and solution techniques in COMMIX are entirely general and applicable to other materials (e.g., metals, plastics, composities, etc.) used in several major casting techniques (i.e., investment casting, die casting, injection molding, etc).

The new porous-medium formulation can be viewed as an approximation of irregular geometries which are often encountered in casting molds. This formulation is particularly suitable for the marshy zone where dendrites may be modeled using the concept of volume porosity and directional surface porosity in fluid flow calculations. It appears that the new porous-medium formulation presented here is very advantageous for casting modeling and has been proven to be numerically very efficient.

The method described in this paper represents a state-of-the-art of fluid flow and heat transfer modeling of the casting process. Although a great deal of additional modeling work is needed however, the work presented here should serve as a foundation for future generic casting modeling.

A number of phenomenological models in casting processes should be investigated and implemented in the COMMIX code. These models are natural convection of liquid melt, air entrainment, phase transformation, interface stability, mechanisms of formation of dendrite, nucleation, and micro- and macro-segregations, etc.

Finally, it should be pointed out that all phenomenological models should be validated with appropriate separate experiments and COMMIX results should be validated with integral experiments under a variety of operating conditions.

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